Rad. and Environm. Biophys. 12, 321—335 (1975)

Concepts of Microdosimetry*

III. Mean Values of the Microdosimetric Distributions

A. M. Kellerer and D. Chmelevsky**

Department of Radiology, Radiological Research Laboratory, College of Physicians and Surgeons, Columbia University, New York

Received August 5, 1975

Summary. This is the last part of an investigation of microdosimetric concepts relevant to numerical calculations. A formula is derived which permits the computation of the dose average lineal energy, $\bar{y}_D$, or the corresponding average of the specific energy without the need to determine the probability distributions, $f(y)$ or $f_1(z)$. A detailed treatment is given for two cases of practical importance. The first case corresponds to spherical sites with diameters of the order of 1 μm and to neutrons up to 15 MeV. The second case corresponds to microscopic sites which are small enough that the change of the stopping power of charged particles traversing the site can be neglected.

Introduction

Two earlier articles [14, 15] have dealt with established microdosimetric quantities [10, 18, 27, 28] and with sampling procedures which lead from simulated particle tracks [24 to 26] to the probability distributions of these quantities and to their mean values. Such sampling, like all Monte Carlo procedures, may require extensive computations for sufficient statistical accuracy. In this last part of the study a formula is derived which permits the direct calculation of $\bar{y}_D$ without the necessity to compute the explicit probability distribution $f(y)$. This possibility is important because the quantity $\bar{y}_D$ is particularly relevant to theoretical radiation biology [19]. We refer mainly to the quantity $\bar{y}_D$ which is the microdosimetric analogon to the dose average, $\bar{L}_D$, of linear energy transfer. However it will be understood that all considerations apply equally to the closely related quantity $\bar{z}_{D1}$.

The formula will permit the numerical determination of $\bar{y}_D$ from simulated random tracks without the need to apply sampling procedures. This is the case of principal interest in the present context; it will therefore be discussed in detail. In certain cases the formula can also yield direct analytical expressions for $\bar{y}_D$ so that no simulated particle tracks are needed. The condition for this possibility is that one deals with sites which are large enough that energy-loss straggling and the finite range of δ-rays in the particle tracks can be neglected. The most important practical case where this condition is met is that of intermediate energy neutrons and of sites not much smaller than 1 μm [3, 4]. Equations which apply to this

* This investigation was supported by Contract AT(11-1)3243 from the United States Atomic Energy Commission and Public Health Service Research Grants No. CA 12536 and CA 15307 from the National Cancer Institute.

** Present address: Centre d'Etudes Nucléaires, DPr/Sps, Fontenay-aux-Roses, France.

situation will be given. Except for some illustrative examples no numerical evaluations will be presented. Some numerical results have been given in a preliminary report [17].

Apart from the dose average $\bar{y}_D$ one deals in microdosimetry with the frequency average $\bar{y}_F$ and with the corresponding average of specific energy or with its inverse the mean event frequency per unit absorbed dose [18]. The quantity $\bar{y}_F$ is the microdosimetric analogon of the track average, $\bar{L}_T$, of LET. Accordingly it would be desirable to obtain formulae which permit direct numerical derivation of the quantity $\bar{y}_F$ from simulated particle tracks. However we have not found such formulae; it appears that $\bar{y}_F$ has to be derived from simulated particle tracks by such sampling procedures as described in the previous article [15]. The frequency average $\bar{y}_F$ will therefore not be considered in the following. One may however note that simple relations for $\bar{y}_F$ exist in the case of sites large enough that energy-loss straggling and the range of δ-rays can be neglected. These relations and some numerical results have been reported earlier [20].

The Function $T(x)$

In order to derive the formula for $\bar{y}_D$ one needs an auxiliary function. This function will be introduced in the following.

Consider a pattern of energy deposition in a uniform medium exposed to a uniform radiation field. As in the earlier articles this will be called the *inchoate distribution*; it consists of the *transfer points*, T_i, with the corresponding *energy transfers*, ε_i.

Let a transfer point be randomly chosen. Here and in the following the notion of random choice of a transfer point, T_i, is to be understood in the way that the selection probability is proportional to ε_i, *i.e.* it is assumed that the chance of a transfer point to be selected is proportional to the energy transfer, ε_i, belonging to the point. One can then ask for the expected energy imparted within a distance x from the selected transfer point; in the present context this quantity will be called $T(x)$. One can also ask for the expected energy, $t(x)\,\mathrm{d}x$, imparted in a spherical shell of radius x and thickness $\mathrm{d}x$ centered at the transfer point, *i.e.* one can ask for the distribution of imparted energy in distance from a randomly chosen increment, ε_i.

With these definitions one has:

$$t(x) = \frac{\mathrm{d}\,T(x)}{\mathrm{d}x}\,. \tag{1}$$

The two functions have the characteristics of a sum distribution and a differential distribution; however they are not normalized[1].

The function $T(x)$ can be split into two separate components. The first component which one might call $T_1(x)$ includes the contributions from the same particle track as the reference point. The second component includes the con-

[1] Since the symbol for the function is always accompanied by its argument there will be no possibility of confusion between $T(x)$ and the symbol, T_i, for transfer points.

According to the terminology used in the Appendix of the preceding article $T(x)$ could be written $\bar{\varepsilon}_C$, *i.e.* $T(x)$ is the mean value of the centered distribution, $c(\varepsilon)$, of energy imparted for a sphere radius x. The explicit distribution $c(\varepsilon)$ will not be required in the following. The symbols $T(x)$ and $t(x)$ are used in order to simplify the notation.

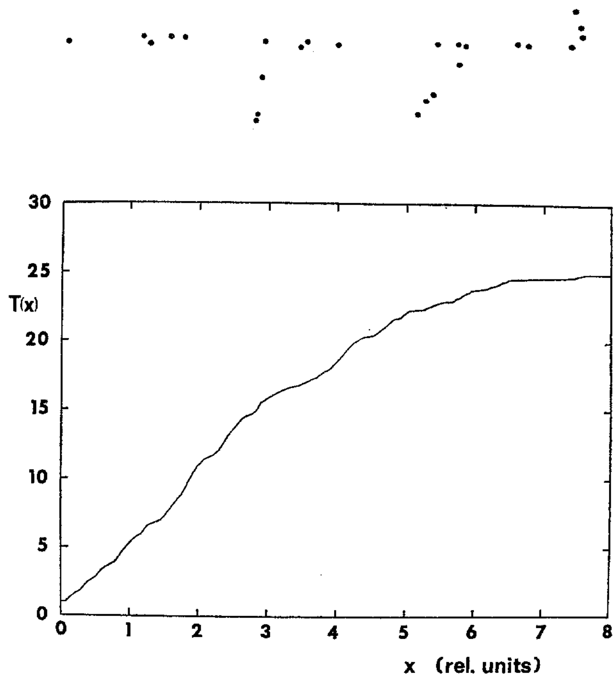


Fig. 1. Schematic example of a microscopic pattern of energy deposition and the function $T(x)$ which results if all dots are assumed to represent unit energy transfer. $T(x)$ is the expected number of transfers within a circle of radius x centered at a randomly selected transfer. The function can also be considered as the sum distribution of distances between pairs of transfer points multiplied by the total number of transfer points

tributions from independent particle tracks. These latter contributions are not spatially correlated to the reference point and are therefore simply proportional to absorbed dose:

$$T(x) = T_1(x) + \frac{4\pi\varrho}{3} x^3 D. \tag{2}$$

An analogous equation applies to the derivative:

$$t(x) = t_1(x) + 4\pi\varrho x^2 D, \tag{3}$$

where ϱ is the density of the medium.

Since the contribution to $T(x)$ from independent particle tracks is a trivial term which is independent of radiation quality and simply proportional to absorbed dose, it will in the following not be considered. The discussion will therefore be concerned solely with the functions $T_1(x)$ and $t_1(x)$ which refer to individual particle tracks. For convenience the index 1 will be dropped.

From the definition of the function one obtains the following expression which permits the derivation of $T(x)$ from an inchoate distribution:

$$T(x) = \sum_{(i,k)<x} \varepsilon_i \varepsilon_k / \sum_i \varepsilon_i . \tag{4}$$

The first sum extends over all pairs of transfer points, T_i and T_k, whose distance, (i, k), does not exceed x. The sum in the denominator extends over all transfer points.

Although this is somewhat arbitrary it is assumed that the contribution of each transfer point itself is included in the sum, *i.e.* the combinations $i = k$ are included in Eq. (4). For $i \neq k$ each pair of points appears twice in the sum, namely in the combinations i, k and k, i.

The numerical evaluation of Eq. (4) is much simpler than the procedure which leads to the explicit distribution of y because it involves the evaluation of only a finite number of terms and does not require random sampling. Although for large simulated particle tracks and for large values of x the number of terms can be considerable, it is usually not prohibitive.

$T(x)$ can be considered as the sum distribution of distances between all energy transfers in a particle track. It is an interesting, although apparently unsolved, problem whether this function determines the random track, *i.e.* whether one can reconstruct a particle track if the functions $T(x)$ or $t(x)$ are precisely known [13]. The problem is however not directly relevant to the present discussion.

As a simple illustration Fig. 1 represents the function $T(x)$ for the same schematic example invoked in the earlier articles [14, 15]. Numerical examples for protons and for fast electrons are given in Appendix A which contains a brief discussion of the direct radiobiological applicability of the function $T(x)$.

The Formula for $\bar{y}_D$

Assume that a transfer point, T_i, is randomly selected on a charged particle track. Then consider all possible spheres, S, of radius r which contain T_i. According to the procedure which in the preceding article [15] has been termed *sampling over individual transfers* the expected energy imparted in a sphere S is equal to $\bar{\varepsilon}_{D1}$. The latter quantity is equal to $\frac{4}{3} r \bar{y}_D$.

The expected energy in a spherical shell of radius x and thickness $\mathrm{d}x$ centered at T_i is $t(x)\,\mathrm{d}x$. One must ask for the expected fraction of this energy which will appear in a sphere S, *i.e.* one needs to know the probability that a point at a distance x from T_i lies in S. This probability is equal to the probability, $U(x)$, that starting in a random direction from a random point in a sphere of radius r one will cover a distance larger than x till leaving the sphere. This is the sum distribution of chord lengths for so-called *internal source randomness* (see [12]) and from a general formula given for this distribution (see Eq. (7) of [12]) one obtains in the special case of a sphere:

$$U(x) = 1 - \frac{3x}{4r} + \frac{x^3}{16r^3}; \qquad 0 \leq x \leq 2r. \tag{5}$$

That part of the expected energy at a distance between x and $x + \mathrm{d}x$ from T_i which is also inside the sphere S is $U(x)\,t(x)\,\mathrm{d}x$. Accordingly one has:

$$\bar{\varepsilon}_{D1} = \int_0^{2r} U(x)\,t(x)\,\mathrm{d}x. \tag{6}$$

The dose average of lineal energy is therefore:

$$\bar{y}_D = \frac{3}{4\,r} \int_0^{2r} \left(1 - \frac{3\,x}{4\,r} + \frac{x^3}{16\,r^3}\right) t(x)\,\mathrm{d}x. \tag{7}$$

The equation for $\bar{z}_{D1}$ is analogous.

It must be kept in mind that the proof of these relations requires a uniform radiation field. In the case of a non-uniform field the relations will still hold if the site is randomly positioned throughout the medium.

This concludes the derivation of the essential result. The remainder of the article consists of a more detailed analysis in special situations.

In Appendix B Eq. (6) is put into a more general context.

Consideration of Special Cases

The formula for $\bar{y}_D$ is of general applicability since $t(x)$ can be calculated for any inchoate distribution. However under certain conditions the theoretical treatment can be carried further. Two such cases will be considered. The first case is that of regions large enough that the internal structure of particle tracks can be neglected, and the tracks can be considered as straight line segments without radial extension. The second case is that of regions small enough that the change of energy of the charged particles traversing these regions can be neglected. This second situation will be treated in more detail because it includes those cases to which microdosimetric techniques are not yet applicable.

Large Sites

Under certain conditions one can neglect both energy-loss straggling and the radial extension of particle tracks. The range of applicability of this simplification has been assessed earlier [16]. In the present context it is sufficient to point out that energy-loss straggling and radial extension of the tracks can be disregarded if one deals with sites not much smaller than 1 µm and with moderately fast heavy charged particles such as the recoils of neutrons of energy up to about 15 MeV. Caswell and Coyne have utilized this fact in extensive computations of microdosimetric distributions [3, 4]. Formulae for $t(x)$ and $\bar{y}_D$ in this particular case will be derived.

One may first consider an oversimplification, namely that of straight particle tracks without radial extension and with a continuous and constant rate of energy transfer, L. In this case one has:

$$t(x) = 2\,L. \tag{8}$$

The value $\bar{y}_D$ which results in this case is well known. Nevertheless it is instructive to consider its derivation from the distance distribution. According to Eq. (7) one has:

$$\bar{y}_D = \frac{3}{4\,r} \int_0^{2r} \left(1 - \frac{3\,x}{4\,r} + \frac{x^3}{16\,r^3}\right) 2\,L\,\mathrm{d}x = \frac{9}{8}\,L. \tag{9}$$

Naturally this is an undue simplification. For a more realistic treatment one may consider a particle of specified energy, E. As before, the particle track will be approximated by continuous energy transfer along straight lines. However the finite range, R, of the particle and the change of linear energy transfer along the track will be taken into account. To indicate the dependence on the initial energy, E, of the particle the notation $t_E(x)$ and $\bar{y}_{D,E}$ will be used.

Let E_s and L_s be the energy and the stopping power of the particle as functions of its remaining range, s. Then according to the definition of $t(x)$ one obtains:

$$t_E(x) = \frac{2}{E} \int_x^R L_{s-x} \, L_s \, \mathrm{d}s. \tag{10}$$

As pointed out R is the initial range of the particle and E is its initial energy. If one were to assume constant stopping power, L, along the particle track one would obtain:

$$t_E(x) = 2\,L\left(1 - \frac{x}{R}\right). \tag{11}$$

In reality one must perform the integration for the actual variation of LET along the particle track.

The dose mean lineal energy, $\bar{y}_{D,E}$, for a proton of energy E is, according to Eq. (7):

$$\bar{y}_{D,E} = \frac{3}{4\,r} \int_0^{2r} \left(1 - \frac{3\,x}{4\,r} + \frac{x^3}{16\,x^3}\right) t_E(x) \, \mathrm{d}x. \tag{12}$$

The corresponding quantity for the recoil particles produced by neutrons can be obtained by averaging the quantity $\bar{y}_{D,E}$ over all initial energies and all types of recoil particles. For simplicity we will confine the discussion to one type of particles, namely the recoil protons. It will be obvious how the formulae are to be modified in the general case.

Assume that $p(E)\,\mathrm{d}E$ is the fraction of protons with initial energy between E and $E + \mathrm{d}E$. Then the fraction of absorbed dose contributed by these particles is proportional to $E\,p(E)\,\mathrm{d}E$, and one obtains therefore:

$$\bar{y}_D = \int_0^{E_{\max}} \bar{y}_{D,E} \, E \, p(E) \, \mathrm{d}E \,/\, \overline{E}, \tag{13}$$

where $\overline{E} = \int_0^{E_{\max}} E\,p(E)\,\mathrm{d}E$ is the mean initial proton energy.

Therefore, if proton recoils from monoenergetic neutrons are equi-distributed in energy, *i.e.* if $p(E) = 1/E_n$ up to the energy, E_n, of the neutrons:

$$\bar{y}_D = \frac{2}{E_n^2} \int_0^{E_n} \bar{y}_{D,E} \, E \, \mathrm{d}E \,. \tag{14}$$

The same result can be obtained by a second method which is somewhat more convenient because it does not require three successive integrations. This method is to derive the function $t(x)$ directly for the mixed field of recoil protons, and then to derive the quantity $\bar{y}_D$. For $t(x)$ one has:

$$t(x) = \int_0^{E_{\max}} t_E(x) \, E \, p(E) \, \mathrm{d}E \,/\, \overline{E}. \tag{15}$$

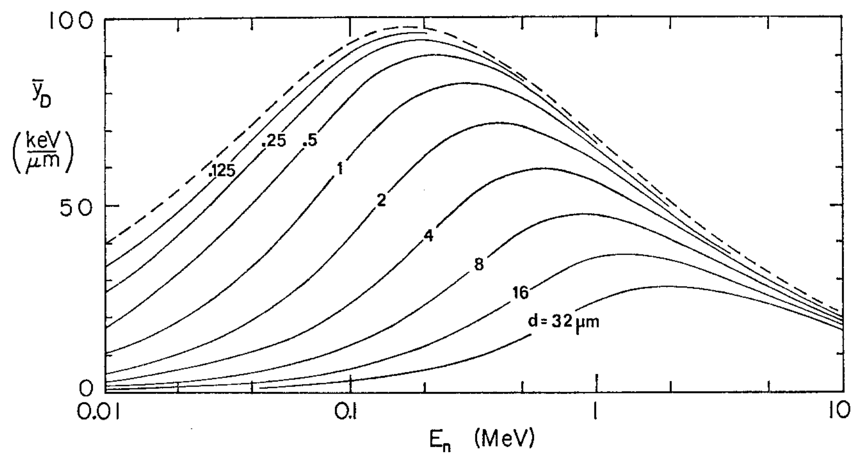


Fig. 2. Dose mean lineal energy, $\bar{y}_D$, for the recoil protons produced by monoenergetic neutrons. The diameter, d, of the spherical site is given as a parameter of the curves. The ranges and stopping powers are those given in ICRU Report 16 for water [9]. The broken line corresponds to the value 9/8 $\bar{L}_D$ [see Eq. (9)]

Using Eq. (10) one obtains:

$$t(x) = \frac{2}{\bar{E}} \int_x^{s_{max}} L_{s-x}\, L_s\, P(s)\, ds. \tag{16}$$

$P(s)$ is the fraction of recoils with initial range larger than s and s_{max} is the range at maximum recoil energy. The quantity $\bar{y}_D$ then results from Eq. (7). Fig. 2 represents as an example numerical results for the proton recoils of mono-energetic neutrons. Equi-distribution of energy is assumed for the recoils.

Small Sites

Assume that a charged particle traverses a microscopic volume or passes the volume at such a distance that it can inject δ-rays into it. If the volume is small enough and the particle is of sufficient energy then the change of its kinetic energy during the process can be neglected, *i.e.* one deals with track segments of constant linear energy transfer. In the following such track segments will be considered. The term *small sites* may be used to refer to the situation. Accordingly, when in this section the functions $T(x)$ and $t(x)$ and the lineal energy averages $\bar{y}_D$ are referred to, they belong to a specified particle at a specified energy. This must be distinguished from the convention in the preceding section where the quantities belonged to the total track of a particle with specified energy.

Various quantities, in addition to LET, can be used to characterize a short track segment. One of the important factors is the relative frequency of δ-rays of various energies generated along the track segment. The term δ-ray is here used in the general sense of a collison event of the primary particle; in contrast to the more common usage it stands therefore not only for events in which an ionizing recoil electron is produced but it applies also to collisions which result only in a single ionization or even excitation. To a first approximation one can assume that the spectrum of δ-rays depends only on the velocity of a heavy charged particle. This will be the essential point in the present context; it will not be necessary to make specific assumption on the actual form of the δ-ray spectrum.

Another function relevant to the description of a particle track is the distribution of energy in distance, b, from the particle track. This function which characterizes the average radial profile of the track has been extensively discussed in the literature [2, 5, 6, 11, 24, 29] and has for protons up to 3 MeV been experimentally determined [1, 29]. Let $G(b)$ be the fraction of energy which is imparted at a distance from the track core less than b. It is assumed that this function is normalized to $G(\infty) = 1$. In addition one may use the derivative, $g(b)$:

$$g(b) = \frac{\mathrm{d}G(b)}{\mathrm{d}b} \tag{17}$$

$g(b)\,\mathrm{d}b$ is the expected fraction of energy deposited in a cylindrical shell of radius b and thickness $\mathrm{d}b$ whose axis is the track core. The functions $G(b)$ and $g(b)$ will be referred to as *radial energy distributions*. They will be used as auxiliary functions; it is important to realize that they are only statistical averages and do not determine the actual energy concentrations around the track.

One may note that the quantity $G(b)$ is equal to the linear energy transfer, L_b, with distance cut-off [9] divided by the total linear energy transfer, L:

$$G(b) = L_b/L. \tag{18}$$

The absorbed dose at a distance b from the track core is:

$$D_b = L\,g(b)/2\pi b. \tag{19}$$

It is frequently assumed that outside the track-core and up to a certain maximum value of b the function $g(b)$ is inversely proportional to b. However the present considerations apply regardless of the form of the function $g(b)$.

A general property of the functions $T(x)$ and $t(x)$ and the quantity $\bar{y}_D$ can be derived from the fact that the spectrum of δ-rays and the radial energy distribution depend only on the velocity of the heavy charged particle. The following considerations will apply to heavy charged particles of specified velocity but of different charge and therefore of different linear energy transfer, L.

$T(x)$ is the expected energy in a sphere of radius x centered at a randomly selected transfer point in the track. This expected energy can be split into two separate components. The first component, $T_\delta(x)$, includes the contributions from the same δ-ray that has produced the transfer. This component depends only on the spectrum of δ-rays and not on the linear energy transfer, L. The second component includes the contribution from separate δ-rays. This contribution is, for particles of equal velocity, proportional to L. This follows from the fact that a larger charge of the particle leads not to different δ-rays but only to a higher average frequency of δ-rays per unit track length. Accordingly one can write:

$$T(x) = T_\delta(x) + T_a(x)\,L. \tag{20}$$

The term $T_a(x)\,L$ is equal to the value $T(x)$ which would result if the association of energy in δ-rays could be neglected [2]. In other words, $T_a(x)\,L$ would result if one

[2] The quantity $T_a(x)$ refers to unit linear energy transfer, therefore its dimension is different from that of $T(x)$. Analogous remarks apply to the quantities $t_a(x)$ and $\bar{y}_a$.

were to deal with a track with no internal structure but with a radial energy distribution which is equal to that of the actual track. Such a simplified track results if one averages out the energy concentration in cylindrical shells around the particle track. In the following the term *amorphous track* will be used to refer to this simplification. The index a in the function $T_a(x)$ refers to this expression.

An analogous equation applies to the derivative $t(x)$:

$$t(x) = t_\delta(x) + t_a(x)\, L \tag{21}$$

and, by virtue of Eq. (7), also to the dose mean lineal energy, $\bar{y}_D$:

$$\bar{y}_D = \bar{y}_\delta + \bar{y}_a\, L. \tag{22}$$

This equation establishes a connection between the values $\bar{y}_D$ for different heavy charged particles of the same velocity; it can therefore serve as a check of experimental microdosimetric data. It also provides a criterion for the possibility to assume an amorphous track, *i.e.* to disregard the local concentration of energy in δ-rays. The criterion is that $\bar{y}_\delta$ is small as compared to $\bar{y}_a\, L$.

Although no numerical evaluation will be presented in this article, it is useful to consider the derivation of the quantities appearing in Eqs. (20 to 22). Only the essential formulae will be given.

The terms $T_\delta(x)$, $t_\delta(x)$, or $\bar{y}_\delta$ can be derived by sampling simulated δ-rays which correspond to the particle velocity which is being studied. It is sufficient to derive $T_\delta(x)$ according to Eq. (4). Then $t_\delta(x)$ is obtained as the derivative of $T_\delta(x)$, and $\bar{y}_\delta$ results from Eq. (7). Alternatively one may determine $T_\delta(x)$, $t_\delta(x)$ or $\bar{y}_\delta$ as functions of the energy of δ-rays and then integrate the resulting function over the δ-ray spectrum.

It is of interest to note that the angular distribution of the emission of the δ-rays does not affect the quantity $\bar{y}_\delta$. The angular distribution enters the calculations only insofar as it influences the radial energy distribution and thereby the second terms in Eqs. (20 to 22). Since the radial energy distribution may be experimentally determined [1, 29] one can arrive at the values of $\bar{y}_D$ or of the distance distribution without knowledge of the angular distribution of δ-rays.

For the derivation of $T_a(y)$ one needs a function, $T_{bb'}(x)$, which is defined in the following way. Assume an infinite cylinder of radius b' and a point at a distance b from the axis of the cylinder. Then $2\pi b'\, T_{bb'}(x)$ is the surface of the cylinder which lies inside a sphere of radius x centered at the point. One obtains:

$$T_{bb'}(x) = \frac{2}{\pi} \int_0^\pi \sqrt{x^2 - b^2 - b'^2 + 2\, bb' \cos\phi}\; \mathrm{d}\phi; \qquad x > |\, b - b'\,|. \tag{23}$$

The quantity $T_a(x)$ results from an integration over all pairs of values b and b':

$$T_a(x) = \int_0^\infty \int_0^\infty T_{bb'}(x)\, g(b)\, g(b')\, \mathrm{d}b\, \mathrm{d}b'. \tag{24}$$

The function $t_a(x)$ is obtained as the derivative of the sum distribution, and $\bar{y}_a$ is calculated according to Eq. (7).

These are the essential formulae which determine the quantity $\bar{y}_D$ for small sites. In conclusion we will consider a special situation which corresponds to recent microdosimetric measurements [7, 8, 22, 23]. These measurements have

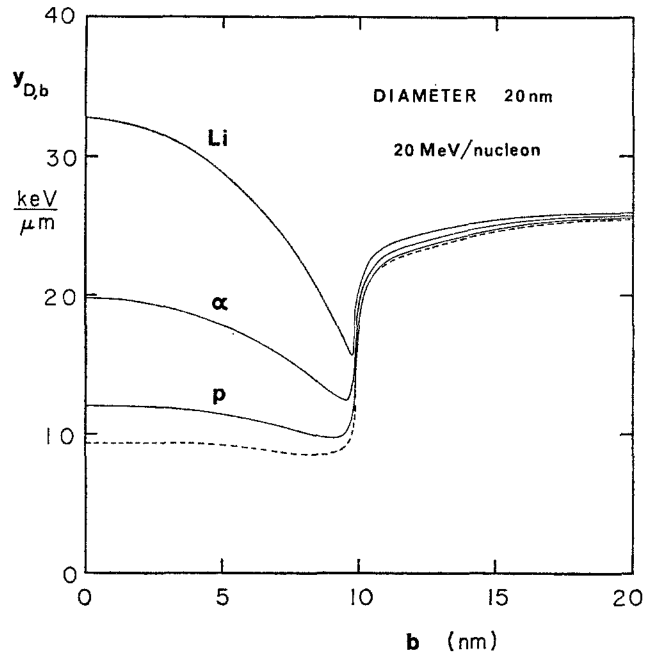


Fig. 3. The dose mean lineal energy, $\bar{y}_{D,b}$, for a spherical site of 10 nm radius and a collimated beam of heavy particles. The parameter b is the distance between the particle beam and the center of the sphere. The solid curves refer to protons, alpha particles, and lithium ions with energy of 20 MeV per nucleon. The values are interrelated according to Eq. (25). The term $\bar{y}_{\delta,b}$ is indicated as a broken line. The data have been computed from simulated proton tracks created by H. G. Paretzke. The stopping powers are those for water

been performed with a collimated beam of charged particles passing at a distance, b, from the center of a spherical [8, 22, 23] or cylindrical [7] wall-less proportional counter. This situation is more complicated than the cases treated earlier. The reason is that one deals not with a uniform radiation field, and that one can consequently not apply the relation between $t(x)$ and $\bar{y}_D$. Nevertheless one obtains an equation which is analogous to Eq. (22). This can be seen in the following way.

The core of the particle track is at a distance b from the center of the sphere. In the computational approach one must therefore sample the value of y only on the surface of a cylinder of radius b around the track. Taking this condition into account one can apply a procedure which corresponds to the sampling over individual transfers described in the preceding article [15]. As in earlier derivations one can split the value of y at a sampling point into two contributions. The first contribution is from the same δ-ray to which the selected transfer belongs; this term depends only on the spectrum of δ-rays, *i.e.* on the velocity of the primary particle. The second contribution belongs to independent δ-rays and is therefore proportional to the linear energy transfer. One obtains therefore a relation which corresponds to Eq. (22):

$$\bar{y}_{D,b} = \bar{y}_{\delta,b} + \bar{y}_{a,b}\, L\,. \qquad (25)$$

The index b is used to indicate that the quantities relate to a fixed impact parameter, b, of the charged particles.

The term $\bar{y}_{a,b}\, L$ is equal to $3\,\langle\epsilon_b\rangle/4\,r$, where $\langle\epsilon_b\rangle$ is the expected energy imparted to the spherical site per particle passing it at distance b:

$$\langle\epsilon_b\rangle = L \int_c^{b+r} T_{bb'}(r)\, g(b')\, \mathrm{d}b', \tag{26}$$

where the lower limit, c, of the integration is 0 for $b \leq r$ and $b - r$ for $b > r$. One must note that the average $\langle\epsilon_b\rangle$ includes those cases where $\epsilon = 0$.

$\langle\epsilon_b\rangle$ decreases sharply when b becomes larger than r, and when accordingly the particle passes outside the sphere. In contrast $\bar{y}_{\delta,b}$ increases sharply as b becomes larger than r. The reason is that for $b < r$ collisions of the charged particle which result in small energy transfers such as single ionizations or excitations influence $\bar{y}_{\delta,b}$, while for $b > r$ only higher energy δ-rays which enter the sphere are involved. This can lead to the somewhat surprising result that $\bar{y}_{D,b}$ has its smallest value when the particle passes at very close distance from the site, while its value is larger both for direct traversals and for passages at larger distance from the site. Fig. 3 illustrates this by an example from unpublished calculations. The example refers to small sites of 20 nm diameter; measurements for sites of 1 μm diameter have shown the same characteristics [7, 8, 22, 23].

Acknowledgement. The concepts developed by Dr. H. H. Rossi have been the basis of this study; his advice and his criticism were equally essential.

We are grateful to Dr. H. G. Paretzke for providing us with simulated particle tracks. The examples used to illustrate this article reflect only a minor part of his extensive data. We are also indebted to Dr. A. V. Kuehner for his help with the numerical evaluations.

Appendix A:

Applications of the Functions $T(x)$ and $t(x)$

$T(x)$ and its derivative, $t(x)$, have been introduced as auxiliary functions in the formula for $\bar{y}_D$. However the functions have also direct radiobiological implications. This may be demonstrated by an example.

Assume that DNA single-strand breaks result in an irradiated medium with probability $\alpha\varepsilon_i$ at any point where an energy transfer, ε_i, occurs. Assume further that pairs of these breaks have a probability $p(x)$ to cause a double-strand break which depends on their spatial separation x. One then obtains the following equation for the yield, $E(D)$, per unit volume of double-strand breaks at the absorbed dose D:

$$E(D) = \frac{\alpha^2}{2} D \left(\int_0^\infty p(x)\, t(x)\, \mathrm{d}x + 4\,\pi\,\varrho \int_0^\infty x^2\, p(x)\, \mathrm{d}x\, D \right) = k\,(\xi\, D + D^2) \tag{A.1}$$

with:

$$\xi = \int_0^\infty p(x)\, t(x)\, \mathrm{d}x \,/\, 4\,\pi\,\varrho \int_0^\infty p(x)\, x^2\, \mathrm{d}x. \tag{A.2}$$

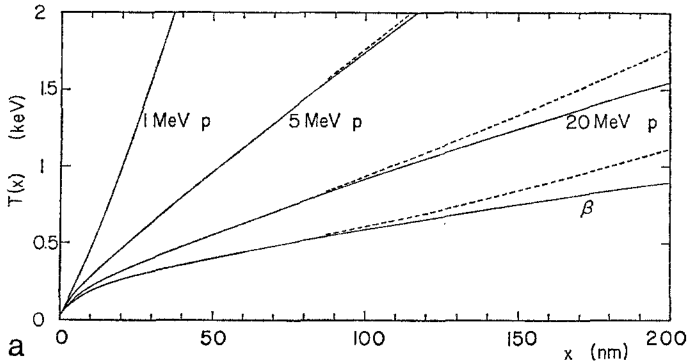
One could make the simple assumption that two single-strand breaks have a fixed probability to cause a double-strand break if separated by a distance less than r:

$$p(x) = \begin{cases} p \text{ for } x < r \\ 0 \text{ for } x > r \end{cases} \tag{A.3}$$

with this assumption one obtains:

$$\xi = T(r)/m, \tag{A.4}$$

where m is the mass of a spherical region of radius r.



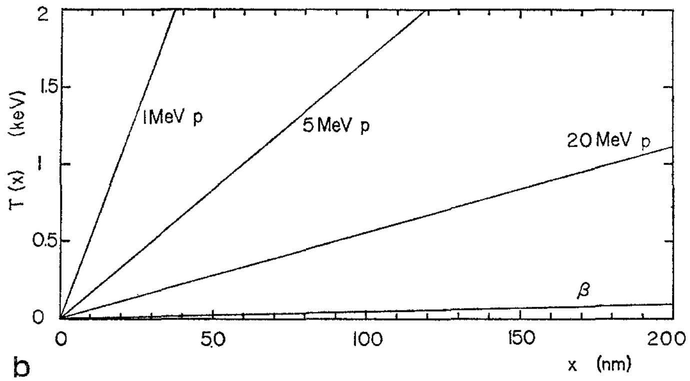


Fig. 4. a) The functions $T(x)$ for proton track segments at various energies, and for fast electrons. The data are derived from simulated particle tracks created by H. G. Paretzke. The stopping powers are those for water. The broken lines indicate those values, $T(x)$, which result if at an absorbed dose of 100 rad the contribution from other particle tracks is included. b) The functions $T(x)$ for protons track segments at various energies and for fast electrons which result if the LET concept is applied, *i.e.* if the formation of δ-rays and the radial extension of the tracks are neglected

If one assumes a more realistic, gradually decreasing function $p(x)$ such as $p\,e^{-x^2/r^2}$ one obtains an expression which is similar to the one in Eqs. (6) and (7):

$$\xi = \frac{1}{\varrho\,\pi^{1.5} r^3} \int_0^\infty e^{-x^2/r^2}\, t(x)\, \mathrm{d}x. \tag{A.5}$$

Fig. 4a represents the quantity $T(x)$ for protons and for values of x up to 200 nm. These results have been obtained from simulated random tracks created by H. G. Paretzke (see [24, 25]). In the present context they merely serve as illustrations; a preliminary report of numerical data has been given earlier [17].

As pointed out $T(x)$ is assumed to refer only to individual particle tracks; *i.e.* $T(x)$ is the expected energy from the *same* particle track in a spherical region of radius x centered at a randomly chosen energy transfer. The functions $T(x)$ which result if, at an absorbed dose of 100 rad, the contribution from other particle tracks is included are inserted as broken lines. It is apparent that the contribution from other particle tracks is insignificant for these small radii. Accordingly the linear term in Eq. (A.1) will be predominant except for large doses or large interaction distances.

Fig. 4b represents the values which result for $T(x)$ if the LET-concept is applied. The comparison of both figures shows that the LET-concept leads to greatly distorted results for low and intermediate stopping powers. Microdosimetric calculations are therefore essential.

Appendix B

General Form of the Equation for $\bar{y}_D$

The formula for $\bar{y}_D$ has been derived for spherical regions. However it is apparent that the proof of Eq. (6) applies to any convex region provided the radiation field is isotropic or the orientation of the region is random. $U(x)$ is the sum distribution of chord lengths for *internal source randomness* [12] for the volume which is being considered.

One may go one step further and generalize Eq. (6) to regions which are not convex or which may even have diffuse boundaries. This generalization will here be mentioned without proof. As pointed out the function $t(x)$ is the product of the total energy transfer in a particle track multiplied by the probability density of distances between two randomly selected energy transfers in the track. One may define an analogous function for the site. Let $t'(x)$ be the product of the volume of the site and the probability density of distances x between two randomly selected points in the site. One can also say that $t'(x)\,dx$ is the expected volume of the site which lies inside a spherical shell of radius x and thickness dx centered around a point randomly chosen in the site. One finds that Eq. (6) can then be written in the form:

$$\bar{\varepsilon}_{D1} = \int_0^\infty t(x)\, t'(x)/4\,\pi\, x^2\, dx \tag{B.1}$$

This more symmetrical form of the equation makes it clear that it refers to the general mathematical problem of the random intersection of two geometrical objects, namely the particle track and the site.

The function $t'(x)$ for a sphere can be obtained from the formula for hyper-spheres given by Kendall and Moran [21]. Comparison of Eqs. (6) and (B.1) shows that $t'(x) = 4\,\pi\, x^2\, U(x)$.

One may use the generalized formula to obtain the mean values $\bar{z}_{D1}$ which apply to a blurred site. This is of particular interest because, as found in the earlier article [14], the values of z for a blurred site are equal to the values of z which occur in infinitesimally small sites if a diffusion process corresponding to the radial profile of the blurred site is applied to the imparted energy.

Assume that the site is of spherical symmetry but has a density which decreases as e^{-x^2/r^2}, where x is the distance from the center. One finds, and the proof is omitted here, that the function $t'(x)$ for such a body is:

$$t'(x) = 4\,\pi\, x^2\, e^{-x^2/2r^2}. \tag{B.2}$$

With Eq. (B.1) and with Eq. (5) of the earlier article [14] one obtains:

$$\bar{z}_{D1} = \frac{1}{\varrho\, \pi^{1.5}\, r^3} \int_0^\infty t(x)\, e^{-x^2/2r^2}\, dx. \tag{B.3}$$

This corresponds to the equation:

$$\bar{z}_{D1} = \frac{3}{\varrho\, 4\,\pi\, r^3} \int_0^{2r} t(x) \left(1 - \frac{3\,x}{4\,r} + \frac{x^3}{16\,r^3}\right) dx \tag{B.4}$$

which applies to a sphere of radius r. That the two equations must result in values $\bar{z}_{D1}$ of the same order of magnitude can be seen from the comparison of the two functions

$$c_1 = \frac{1}{\pi^{1.5}}\, e^{-x^2/2} \tag{B.5}$$

and

$$c_2 = \frac{3}{4\,\pi} \left(1 - \frac{3\,x}{4} + \frac{x^3}{16}\right) \tag{B.6}$$

which are plotted in Fig. 5.

One concludes that similar values $\bar{z}_{D1}$ are obtained for the mean specific energy in a spherical site of radius r, for the mean specific energy in a blurred site of effective radius r, and for the

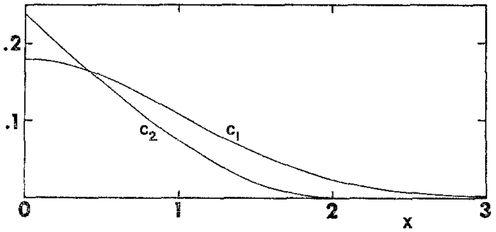


Fig. 5. Comparison of the quantities c_1 and c_2 in Eqs. (B.5) and (B.6)

mean specific energy in infinitesimal sites after diffusion of the imparted energy over the effective distance r. The quantity $\bar{z}_{D1}$ is therefore a very general parameter of radiation quality.

References

1. Baum, J. W.: Comparison of distance- and energy-restricted linear energy transfer for heavy particles with 0.25 to 1000 MeV/AMU. In: Proceedings of 2nd Symposium on Microdosimetry (Ebert, H. G. *Ed.*) pp. 653—666. Euratom, 4452 d-f-e (1970)
2. Berger, M. J.: Some new transport calculations of the deposition of energy in biological materials by low-energy electrons. In: Proceedings of 4th Symposium on Microdosimetry (Ebert, H. G., *Ed.*) pp. 695—715. Euratom 5122 d-e-f (1974)
3. Caswell, R. S.: Deposition of energy by neutrons in spherical cavities. Radiat. Res. **27**, 92—107 (1966)
4. Caswell, R. S., Coyne, J. J.: Secondary particle spectra produced by neutron interactions with tissue. In: Proceedings of 1st Symposium on Neutron Dosimetry in Biology and Medicine (Burger, G., Schraube, H., Ebert, H. G., *Eds.*). pp. 25—41. Euratom, 4896 d-f-e (1972)
5. Chatterjee, A., Maccabee, H., Tobias, C.: Radial cut-off LET and radial cut-off dose calculations for heavy charged particles in water. Radiat. Res. **54**, 479—494 (1973)
6. Fain, J., Monnin, M., Montret, M.: Energy density deposited by a heavy ion around its path. In: Proceedings 4th Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 169—188. Euratom d-e-f (1974)
7. Glass, W. A., Roesch, W. C.: Measurement of ionization distributions in tissue-equivalent gas. Radiat. Res. **49**, 477—494 (1972)
8. Gross, W., Rodgers, R. C.: Heavy ion event spectra. In: Proceedings of 3rd Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 873—887. Euratom 4810 d-f-e (1972)
9. ICRU: Linear Energy Transfer, Report 16. Washington, D.C.: International Commission of Radiation Units and Measurements 1970
10. ICRU: Radiation Quantities and Units, Report 19. Washington, D.C.: International Commission of Radiation Units and Measurements 1971
11. Katz, R., Kobetich, E. J.: Particle tracks in condensed matter. In: Charged Particle Tracks in Solids and Liquids (Adams, G. E., Bewley, D. K., Boag, J. W., *Eds.*). pp. 109—119. The Institute of Physics and the Physical Society Conference Series No. 8, London (1970)
12. Kellerer, A. M.: Considerations on the random traversal of convex bodies and solutions for general cylinders. Radiat. Res. **47**, 359—376 (1971)
13. Kellerer, A. M., Bell, W.: Theory of microdosimetry. In: Annual Report on Research Project, USAEC, NYO-2740-7, 73-90 (1970)
14. Kellerer, A. M., Chmelevsky, D.: Concepts of microdosimetry. I. Quantities. Radiat. and Environm. Biophysics **12**, 61—69 (1975)
15. Kellerer, A. M., Chmelevsky, D.: Concepts of microdosimetry. II. Probability distributions of the microdosimetric variables. Radiat. and Environm. Biophysics **12**, 205—216 (1975)
16. Kellerer, A. M., Chmelevsky, D.: Criteria for the applicability of LET. Radiat. Res. **63**, 226—234 (1975)

17. Kellerer, A. M., Chmelevsky, D., Teedla, P.: Numerical derivation of microdosimetric quantities, II. Mean values of the dose distributions. In: Annual Report ERDA No. COO-3243-4, pp. 68—79 (1975)
18. Kellerer, A. M., Rossi, H. H.: Summary of quantities and functions employed in microdosimetry. In: Proceedings 2nd Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 843—853. Euratom 4452 d-f-e (1970)
19. Kellerer, A. M., Rossi, H. H.: The theory of dual radiation action. Current Topics in Radiat. Res. 8, 85—158 (1972)
20. Kellerer, A. M., Rossi, H. H.: Numerical derivation of microdosimetric quantities, I. Mean values of the frequency distributions. In: Annual Report ERDA No. COO-3243-4. pp. 61—67 (1975)
21. Kendall, M. G., Moran, P. A. P.: Geometrical probability. New York: Hafner 1963
22. Kliauga, P., Dvorak, R., Rossi, H. H., Kellerer, A. M.: Microdosimetric distributions as a function of radial distance from heavy ions. In: Annual Report ERDA No. 3243-4, p. 88—103 (1975)
23. Kliauga, P., Rossi, H. H.: Microdosimetric distributions as a function of radial distance from heavy ion tracks. In: Proceedings 5th Symposium on Microdosimetry, Verbania, 1975 (in press)
24. Paretzke, H. G., Leuthold, G., Burger, G., Jacobi, W.: Approaches to physical track structure calculations. In: Proceedings 4th Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 123—140. Euratom, 5122 d-e-f (1974)
25. Paretzke, H. G.: Comparison of track structure calculations with experimental results. In: Proceedings 4th Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 141—168. Euratom, 5122 d-e-f (1974)
26. Patau, J. P., Malbert, M., Terrissol, M., Commanay, L.: Études dosimétriques dans des cavités sphériques situées en milieu semi-infini, irradié par des électrons de 2 MeV. In: Proceedings 4th Symposium on Microdosimetry (Ebert, H. G., *Ed.*). pp. 755—777. Euratom, 5122 d-e-f (1974)
27. Rossi, H. H.: Energy distribution in the absorption of radiation. Advanc. biol. med. Phys. **11**, 27—85 (1967)
28. Rossi, H. H.: Microscopic energy distribution in irradiated matter. In: Radiation Dosimetry (Attix, F. H., Roesch, W. C., *Eds.*), Vol. 1, pp. 43—92. New York: Academic Press 1968
29. Varma, M. N., Baum, J. W., Kuehner, A. V.: Energy deposition by heavy ions in a "tissue equivalent" gas. Radiat. Res. **62**, 1—11 (1975)

Dr. Albrecht M. Kellerer
Institut für Med. Strahlenkunde der Universität
D-8700 Würzburg
Versbacher Landstr. 5
Federal Republic of Germany